Low speed fracture instabilities in a brittle crystal

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When a brittle material is loaded to the limit of its strength, it fails by nucleation and propagation of a crack[1]. The conditions for crack propagation are created by stress concentration in the region of the crack tip and depend on macroscopic parameters such as the geometry and dimensions of the specimen[2]. The way the crack propagates, however, is entirely

determined by atomic–scale phenomena, since brittle crack tips are atomically sharp and propagate by breaking the variously oriented interatomic bonds, one at a time, at each point of the moving crack front[1,3]. The physical interplay of multiple length scales makes brittle fracture a complex "multi–scale" phenomenon, indeed several intermediate scales may arise in more complex situations (e.g. microdefects, grain boundaries). The occurrence of various instabilities in crack propagation at very high speeds is well known[1] and significant advances have been made recently in understanding their origin[4,5]. Here, we investigate low speed propagation instabilities in silicon using quantum–mechanical hybrid multi–scale modelling and single–crystal fracture experiments. Our simulations predict a crack tip reconstruction that makes low–speed crack propagation unstable on the (111) cleavage plane, conventionally thought of as the most stable cleavage plane. We carry out experiments in which this instability is observed for the first time at a range of low speeds, using a novel experimental technique designed for the investigation of fracture under low tensile loads. Further simulations explain why, conversely, at moderately high speeds crack propagation on the (110) cleavage plane becomes unstable and deflects onto (111) planes, as previously observed experimentally.[6,7]

Until relatively recently, the process of brittle fracture has been primarily analysed by continuum mechanics techniques, which predict the driving force for crack propagation—the release of elastic energy per unit advancement as the crack progresses—to be a function of the applied load, the length of the crack, and a geometry dependent factor[1,2,8–10]. The crack is assumed to propagate as long as its energy release rate G is equal to or larger than a material and orientation

dependent critical value. Griffith, who first carried out this analysis, equated the critical energy release rate below which crack propagation cannot take place with the energy 2γ needed to create the new crack surfaces[8]. This approach provides a good description of the fracture process for a straight crack in both static[8] and dynamic regimes[10], as shown by recent experiments on carefully prepared silicon single crystals[7,11–14].

More delicate issues such as the origin of crack path instabilities and materials' resistance to fracture are, however, poorly understood. Even very simple atomistic models show that the discrete nature of the material will manifest itself in a higher resistance to fracture than predicted by Griffith's criterion, due to lattice (or bond) trapping[4,15,16]. This effect depends on the detailed nature of the atomic interactions in the specific material[4,17] and may be very different for different cleavage planes. For a given cleavage plane, it can lead to slow crack growth[1,4,18] and anisotropy with respect to propagation along different crystallographic directions[19,20] or even the sign of the propagation direction[21].

Our simulations use the "Learn–on–the–fly" (LOTF) hybrid classical/quantum–mechanical (QM) molecular dynamics method, which achieves a nearly seamless coupling of the mobile QM and classical regions[22]. We use the QM chemical bonding description where it is necessary near the crack tip but not in the rest of the loaded sample where it is unnecessary and would be prohibitively expensive computationally. We first considered a (111) crack plane with the crack front aligned with the $[1\bar{1}0]$ direction which is under uniaxial $[111]$ tensile load (Fig. 1). Our simulations indicate that the K–field displacement predicted by continuum theory is never stable. Below a load

of $G = 2.1$ Jm^{-2}, much lower than the Griffith critical load ($G = 3.1$ Jm^{-2}, using a value for the surface energy computed with our QM model), the crack closes up. Above this load, a crack tip reconstruction forms spontaneously via a bond rotation (Fig. 1**c**), resulting in the formation of 5– and 7–membered rings (see Supplementary Information). This relieves the stress along the main load axis in the immediate tip region, thus inducing additional lattice trapping. The reconstructed geometry of the crack tip is structurally similar to the Pandey reconstruction of the (111) surface[23]. As such, it could be viewed as the core of a dislocation which remains trapped at the crack tip, unable to induce large scale plasticity at temperatures much lower than the brittle to ductile transition. In simulations performed above the critical load for propagation, the slowly moving $(111)[1\bar{1}0]$ crack occasionally visits the reconstructed tip configuration as it propagates. Remarkably, for slow enough propagation, the $[111]$ oriented bonds in the 6–membered rings located one atomic layer *below* the initial crack plane and further along the propagation direction can break before the bridging bonds associated with the 7–membered ring. Indeed, these are the bonds where the stress is mostly concentrated after the reconstruction. Every such reconstruction and bond breaking event creates a downward $[111]$ step for the system oriented as in Fig. 1**c**, due to the broken mirror symmetry of the crystal. This is at variance with the behaviour expected for propagation at high speeds, larger than those investigated here, where both upwards and downwards steps may occur[24] and macroscopically smooth (111) cleavage surfaces are invariably observed.[25] Our simulations thus predict a systematic deflection of the crack path from the (111) plane at sufficiently low velocities, while fast cracks are dynamically steered away from the instability. We speculate that the deflection process may start with a reconstruction event induced by the local slowing down

of a crack–front segment perhaps due to an encounter with a crystal defect. However started, this process will initiate a positive feedback "sinking" mechanism, since each reconstruction event will further trap and slow down the crack, leading to ever more reconstructions, the whole process yielding observable fracture surface features.

A simple mesoscopic model of the crack tip reconstruction and ensuing feedback process shows how this perturbation can evolve into the macroscopic feature, shown in Fig. 2**d**. A crack front section of length L is modelled by an elastic string[26], represented by a set of N beads, each of mass m, connected by springs. The beads' positions and velocities are represented by the array of dynamical variables $\{\mathbf{r}_i, \mathbf{v}_i\}$, and periodic boundary conditions are imposed in the crack front y direction. The values of most of the parameters in what follows can be directly derived from experimental data, as detailed in the Supplementary Information. The equations of motion for the beads are expressed as a dynamical map[27]:

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \Delta t\, \mathbf{v}_i(t) \tag{1}$$

$$\begin{aligned}\mathbf{v}_i(t+\Delta t) &= \mathbf{v}_i(t) + \frac{\Delta t}{m}\left[f^0\hat{\mathbf{x}} - b\mathbf{v}_i(t) + k[\mathbf{r}_{i+1}(t) + \mathbf{r}_{i-1}(t) - 2\mathbf{r}_i(t)]\right] \\ &\quad -\xi_i \frac{\tau}{l}[v_i^x(t)]^2 + \eta\frac{L}{N}\sum_j \max(0, r_j^x - r_i^x)\end{aligned} \tag{2}$$

$$\xi_i = \frac{s}{1+\exp[(v_i^x - v_0^x)/d]} \tag{3}$$

where Δt is the time step associated with each iteration of the map. Following the order of the right hand side terms of equation (2), the model assumes (i) crack front acceleration in the propagation direction x due to the driving force $f^0\hat{\mathbf{x}}$ induced by the load G, until a limiting speed $v_{\max} = f^0/b$, is reached due to a velocity–dependent phonon drag force $-b\mathbf{v}_i(t)$ with friction coefficient

b; (ii) line tension along the crack front modelled by the springs of strength k; (iii) crack tip reconstruction, occurring at a rate which smoothly rises for decreasing crack speeds, leading to crack climbing by one atomic layer upon each reconstruction, and to slowing of the crack due to reconstruction–induced lattice trapping. This is the key assumption of the model yielding the further drag term quadratic in the velocity, connected with with equation (3) as discussed in detail below; (iv) a driving force increase for crack front sections "held back" during the propagation, to include stress enhancement effects at those segments of the crack which have slowed down and trail behind the rest of the crack front. This leads to extra driving forces for these segments, thus eventually levelling off the ridges. While this last effect is well known, its precise functional form and scaling are not. However, the model is not very sensitive to the details of the stress enhancement term, so that varying its functional form and prefactor η gives rise to only slightly different ridge shapes.

The ξ variable in equation (3) is the local climb slope due to reconstruction, which is velocity dependent. The exact functional form of ξ is again not particularly important, as long as it implies no reconstruction at high velocities (where thus $\xi \approx 0$) and a smooth transition to the maximum observed climb slope s at low velocities. A simple exponential form with scale parameter d which centres the transition on a chosen value $v_0 < v_{\max}$ is used in equation (3), which thus just expresses the fact that climbing results from low propagation speeds, consistent with our calculations and experiments. A macroscopic propagation instability can arise if low propagation speeds can, in turn, be caused by climbing, creating a positive feedback loop, if a perturbation initiates the process by slowing a point of the crack front below a critical speed $v_c < v_{\max}$.

Our simulations provide an atomic scale mechanism leading to such a situation, by revealing that climbing is associated to tip reconstruction events, promoted by low propagation speeds and in turn capable of momentarily trapping and thus locally further slowing down the crack front. In our model we represent this deceleration by imparting a small impulse to the system, directed opposite to the direction of motion, in association with each reconstruction event. If we assume for simplicity that an average of n reconstruction events take place during the time interval Δt for a given bead, its momentum mv will drop by $-n(mv)\tau/\Delta t$, where the parameter $\tau << \Delta t$ is representative of the time delay associated with each reconstruction. The number of events is related to the propagation velocity by $n = \xi v \Delta t/l$, where l is the bilayer distance in the (111) direction, i.e. the amount of climb for each reconstruction event. Thus the momentum change is $-m\xi v^2\tau/l$, which is the nonlinear drag term in equation (2) addressed in point (iii) above. We note that if the frequency of reconstruction events were constant for a given temperature, as is the case for simple activated processes, then ξ would scale as $1/v$, and would just give rise to a simple drag term, linear in the velocity. Thus in an indirect way, this model sheds light on the role of the cooperative, *dynamic* nature of brittle fracture: at high speeds, the atoms near the crack tip are steered towards clean cleavage.

Experimental studies of the low crack–speed regime were performed using a novel technique for applying very small but steady and well controlled tensile loads. The Si specimen is loaded by taking advantage of the thermal expansivity mismatch between the sample and the aluminum loading frame (Fig. 2**b**). Micrographs of the resulting (111) fracture surface are shown in Fig. 2**a**,**c**. Triangular ridges, all deviating in the same direction from the fracture surface, form at a range

of low crack speeds below about 800 ms^{-1}. At higher crack speeds, about 2000 ms^{-1}, the surface is mirror smooth and no ridges are present. The crystallographic direction of the deviation (identical in over 40 independent samples) is the same as the reconstruction–induced steps in the atomistic simulation, and the shape of the ridges is qualitatively in agreement with the mesoscopic model (Figs. 2**c**,**d**). Similar features have recently been reported[25] under more complicated loading conditions at a speed of about 1000 ms^{-1} (see Supplementary Information).

We next considered the (110) crack plane. Experiments have shown that cracks propagating along the $[001]$ direction deflect out of the plane at very low velocity[6,20], while cracks propagating in the $[\bar{1}10]$ direction stay on the (110) plane up to very high velocity (about 2900 ms^{-1}) before also faceting onto (111) planes[6,7]. Recent studies[28] have assigned critical velocities for this instability for various propagation directions and have shown that in all cases the deflection is not immediate but only occurs after some initial propagation on the (110) plane. We simulated the $(110)[\bar{1}10]$ crack propagation and observed the onset of this deflection phenomenon. This crack propagates by breaking a series of bonds labelled A in Fig. 3**a**. The system also contains type B bonds, which are oriented at the same angle with respect to the tension axis as A–bonds. Resolving the elastic stresses on the atomic scale reveals that B–bonds located immediately above and below the crack plane are virtually as highly stressed as A–bonds. However, strong neighbour bonds connecting under–coordinated atoms left exposed by the advancing crack make the A–bonds weaker than B–bonds so that the former are expected to break selectively during quasi–static (110) cleavage, consistent with the low–speed experimental observations.

In the simulations we initially observe each newly exposed under–coordinated surface atom snap back towards the subsurface region. This induces significant local atomic motion while the excess energy diffuses into the bulk crystal, but no immediate rebonding occurs as long as the speed of propagation is sufficiently low. However, bond breaking events become more frequent with increasing crack speed and the local relaxations overlap in time. As more kinetic energy is locally available the fast crack front "stumbles". Local reconstructions involving the removal of under–coordinated atoms begin to occur on the open surfaces. This removes the reason for selective A–bond breaking and in our simulation we indeed observe B–bond breaking events which deflect the crack front onto a (111) plane. Further simulations reveal that under these conditions any slight disturbance away from pure tension (e.g. a small extra shear strain component as in Fig. 3**b**) can systematically reverse the initial relative stability of A– and B–bonds. This results in multiple coherent breaking of B–bonds, effectively exposing (111) surfaces, consistent with the crack motion observed experimentally (Fig. 3**c-e**).

No near–degeneracy of crack tip bonds exists in the orthogonal $[1\bar{1}0]$ direction, consistent with the observation of instabilities only at much higher speeds[6]. The deflection mechanism is thus only operative for the $[001]$ crack propagation direction. In contrast to the (111) cleavage plane, here the formation of new chemical bonds, eventually leading to crack deflection, is favoured by a relatively high propagation speed rather than a low one. This is due to the different interplay between the local atomic motion and the "lattice trapping energy" liberated by the cleavage during the time interval between consecutive crack tip advancement events.

For both cleavage planes in silicon, subtle atomistic details of the crack tip involving dynamical reconstruction mechanisms govern the path of the crack. This is unlikely to be the case for silicon only, due to the general multiscale character of the fracture processes. In the Supplementary Information we present data on preliminary simulations that indicate crack tip reconstruction phenomena in diamond and silicon carbide, and on experiments on sapphire that show low speed instabilities similar to those observed in silicon. Therefore we suggest that crack tip reconstructions occur more generally in brittle solids and control the qualitative macroscopic fracture behavior.

Methods summary

Tensile loading of the silicon (111) system was performed using apparatus shown in Fig. 2**b**. The load is applied by heating the whole setup by a few degrees C. The experimental setup for the (110) system was identical to that in ref. 6. The LOTF hybrid simulations were carried out using a quantum– mechanical model based on density functional theory, as implemented in the CASTEP[29] and SIESTA[30] packages and the Stillinger–Weber potential[31]. The quantum–mechanically treated region was selected automatically during the simulation, based on geometric criteria in relation to the instantaneous crack tip position.

1. Lawn, B. *Fracture of Brittle Solids — Second Edition* (Cambridge Univ. Press, Cambridge, UK, 1993).

2. Broberg, K. B. *Cracks and Fracture* (Academic Press, San Diego, CA, 1999).

3. Lin, I. H. & Thomson, R. Cleavage, dislocation emission, and shielding for cracks under

general loading. *Acta Metall.* **34**, 187–206 (1986).

4. Marder, M. Effects of atoms on brittle fracture. *Int. J. Fract.* **130**, 517–555 (2004).

5. Buehler, M. J. & Gao, H. J. Dynamical fracture instabilities due to local hyperelasticity at crack tips. *Nature* **439**, 307–310 (2006).

6. Sherman, D. & Be'ery, I. From crack deflection to lattice vibrations—macro to atomistic examination of dynamic cleavage fracture. *J. Mech. Phys. Solids* **52**, 1743–1761 (2004).

7. Cramer, T., Wanner, A. & Gumbsch, P. Energy dissipation and path instabilities in dynamic fracture of silicon single crystals. *Phys. Rev. Lett.* **85**, 788 (2000).

8. Griffith, A. A. The phenomena of rupture and flow in solids. *Philos. Trans. R. Soc. London A* **221**, 163 (1921).

9. Irwin, G. R. *Fracturing of Metals*, 147–166 (American Society for Metals, Cleveland, OH, 1948).

10. Freund, L. B. *Dynamic Fracture Mechanics* (Cambridge Univ. Press, Cambridge, UK, 1990).

11. Field, J. E. Brittle fracture: its study and application. *Contemporary Physics* **12**, 1 (1971).

12. Hauch, J. A., Holland, D., Marder, M. P. & Swinney, H. L. Dynamic fracture in single crystal silicon. *Phys. Rev. Lett.* **82**, 3823 (1999).

13. Be'ery, I., Lev, U. & Sherman, D. On the lower limiting velocity of a dynamic crack in brittle solids. *J. Appl. Phys.* **93**, 2429 (2003).

14. Gally, B. J. & Argon, A. S. Brittle-to-ductile transitions in the fracture of silicon single crystals by dynamic crack arrest. *Phil. Mag. A* **81**, 699–740 (2001).

15. Thomson, R., Hsieh, C. & Rana, V. Lattice trapping of fracture cracks. *J. Appl. Phys.* **42**, 3154–3160 (1971).

16. Curtin, W. On lattice trapping of cracks. *J. Mater. Res.* **5**, 1549–1560 (1990).

17. Sinclair, J. E. The influence of the interatomic force law and of kinks on the propagation of brittle cracks. *Philosophical Magazine* **31**, 647–671 (1975).

18. Cook, R. F. & Linegar, E. G. Kinetics of indentation cracking in glass. *J.Am.Ceram.Soc* **76**, 1096–1105 (1993).

19. Riedle, J., Gumbsch, P. & Fischmeister, H. F. Cleavage anisotropy in tungsten single crystals. *Phys. Rev. Lett.* **76**, 3594–3597 (1996).

20. Perez, R. & Gumbsch, P. Directional anisotropy in the cleavage fracture of silicon. *Phys. Rev. Lett.* **84**, 5347–5350 (2000).

21. van Eck, H., van der Laan, D., Dhallé, M., ten Haken, B. & ten Kate, H. Critical current versus strain research at the university of twente. *Supercond. Sci. Technol.* **16**, 1026–1030 (2003).

22. Csányi, G., Albaret, T., Payne, M. & De Vita, A. "learn on the fly": A hybrid classical and quantum-mechanical molecular dynamics simulation. *Phys. Rev. Lett.* **93**, 175503 (2004).

23. Pandey, K. C. New π-bonded chain model for si$(111) - (2 \times 1)$ surface. *Phys. Rev. Lett.* **47**, 1913–1917 (1981).

24. Hoshi, T., Igushi, T. & Fujiwara, T. Nanoscale structures formed in silicon cleavage studied with large-scale electronic structure calculations: Surface reconstruction, steps, and bending. *Phys. Rev. B* **72**, 075323 (2005).

25. Sherman, D., Markovitz, M. & Barkai, O. Dynamic instabilities in 111 silicon. *J. Mech. Phys. Solids* (2007). *in press,* doi:10.1016/j.jmps.2007.05.010.

26. Lange, F. F. The Interaction of a Crack Front with a Second-phase Dispersion. *Philos. Mag.* **22**, 983–992 (1970).

27. Lichtenberg, A. J. & Lieberman, M. A. *Regular and Chaotic Dynamics*, vol. 38 of *Applied Mathematical Sciences* (Springer-Verlag, New York, NY, 1992), 2nd ed. edn.

28. Sherman, D. Macroscopic and microscopic examination of the relationship between crack velocity and path and rayleigh surface wave speed in single crystal silicon. *J. Mech. Phys. Solids* **53**, 2742–2757 (2005).

29. Segall, M. D. *et al.* First-principles simulation: ideas, illustrations and the castep code. *J. Phys.: Cond Mat* **14 (11)**, 2717–2743 (2002).

30. Sanchez-Portal, D., Ordejón, P., Artacho, E. & Soler, J. M. Density-functional method for very large systems with lcao basis sets. *Int. J. Quantum Chem.* **65**, 453 (1997).

31. Stillinger, F. H. & Weber, T. A. Computer simulation of local order in condensed phases of silicon. *Phys. Rev. B.* **31**, 5262 (1985).

32. Kwon, I., Biswas, R., Wang, C., Ho, K. & Soukoulis, C. Transferable tight-binding models for silicon. *Phys. Rev. B.* **49**, 7242 (1994).

33. Sharon, E., Cohen, G. & Fineberg, J. Propagating solitary waves in a rapidly moving crack front. *Nature* **410**, 68–71 (2001).

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Methods

For the (111) system, cleaving of 525 μm thick silicon specimens of 42×26 mm^2 lateral dimensions, cut from a $[110]$ 4" silicon wafer, was performed under tensile load using the apparatus shown in Fig. 2**b**. The specimens were notched with a 150 μm thick diamond saw to a length of 1.5 mm, heated to 200°C and quenched in water to generate a precrack of the required length. The

specimens were then glued to the Al7075 T6 frame using a 150 μm thick film of Epon 815C epoxy resin. The load is applied by heating the whole setup by a few degrees C on a laboratory heating stage due to the difference in thermal expansion coefficients between the sample and the loading frame. When the rate of heating was well below 10°C/min, the instabilities were always present. Using high rates of heating resulted in the propagation of fast cracks leaving behind mirror–smooth surfaces.

In the computer simulations, the CASTEP[29] package was used for the (111) system and the SIESTA[30] package for the (110) system. The classical potential was adjusted to match the linear elastic properties of the quantum–mechanical models in each case. The simulations were carried out in the plane strain configuration and free boundary conditions were used in the x direction. The load, applied by a fixed displacement boundary condition in the y direction, was increased in a number of steps starting from $G = 2.5$ Jm^{-2}, allowing at least 1 ps equilibration time between successive steps, until the crack started to propagate. A variety of strain rates were tested down to 0.1 % ps^{-1}, with no qualitative difference observed. The load needed to crack the system, was 6.0 Jm^{-2} at the lowest strain rate we could afford. Since even at this strain rate the load was found to be still strongly strain rate dependent, this value is only an upper bound. The 300 K constant temperature simulations for the system shown in Fig. 1 were made on a $1200 \times 400 \times 3.8$ Å^3 90868–atom model thin slab, periodic in the crack–front direction. For these low–temperature, highly driven systems, thermal activation and entropy effects, which could induce a qualitatively different behaviour in three–dimensional systems, are unlikely to play a significant role. A series of quasi-static simulations show the same behaviour, although the system has to be overloaded much

more in order to crack, as expected due to the high lattice trapping. In the plane wave DFT part of the LOTF hybrid simulation, the Brillouin Zone was sampled with 4 k–points along the crack front, exchange and correlation were described using the PBE functional, nuclei were described by ultrasoft pseudopotentials, and the electronic wave functions were expanded in plane waves with a 180 eV kinetic energy cutoff. The QM region was selected by an algorithm detailed in the Supplementary Information. The buffer region of the LOTF scheme[22] was set at about 8 Å (4th neighbour distance). Furthermore, we made a test calculation on a 15.2 Å thick slab using a tight binding[32] quantum–mechanical engine to verify that the same phenomena apply in the true three–dimensional case. The reconstruction occurred at all sites along the crack front in quick succession before any other kind of rebonding took place. The simulation of the system shown in Fig. 3 was made on a $687 \times 655 \times 7.6$ Å^3 174752–atom model slab, using the standard SZP basis set with soft confinement for the local orbital DFT part of the calculation. The mesh cutoff was 50 Rydbergs and norm-conserving pseudopotentials were used.

Figure 1 The simulated $(111)[1\bar{1}0]$ crack system. a, Thin strip geometry of the simulation. **b**, Map of the σ_{yy} stress component near the crack tip (red denotes highly stressed, black is unstressed). **c**, Ground state reconstruction geometry of the crack tip under load, created by a rotation of the bond indicated by the arrow. Red atoms are described with quantum mechanics, yellow atoms with an interatomic potential. The small white atoms represent H atoms which we used to terminate the initial surface behind the crack in order to prevent it from closing up at low loads and thereby ease the search for a load value that stabilises the crack (with or without terminating H). The first few bonds that break after the reconstruction are in 6–member rings adjacent to the 7–member ring of the reconstruction. Inset: crack tip structure after reconstruction and subsequent bond breaking. Further increasing the load finally breaks the crack tip bridging bond and advances the open crack surface yielding a downward step in the crack plane (not shown).

Figure 2 Ridges formed by low–speed instabilities on the (111) crack plane. a, Optical micrograph of the (111) crack system. The crack advances from left to right as it accelerates up to a speed of about 800 ms^{-1}, as determined from the faintly visible Wallner lines[33]. The ridges initiate at a variety of crack speeds. **b**, The fracture apparatus, showing the silicon specimen glued to the aluminum frame. **c**, AFM micrograph close–up of a ridge. **d**, Evolution of the crack front with the ridge shape as predicted by a mesoscopic model based on the atomistic reconstruction mechanism illustrated in Fig. 1. The red lines represent snapshots of the propagating crack front yielding the interpolated crack surface (in grey).

Figure 3 The $(110)[1\bar{1}0]$ crack system. **a**, Geometry of the crack tip propagating straight at low speeds by sequential breaking of type A bonds (blue). Red atoms are described with quantum mechanics, yellow atoms with an interatomic potential. At each propagation step, the A–bond is weaker than the corresponding B–bond because of a neighbouring undercoordinated atom (indicated by an arrow for the A_1, B_1 pair). **b**, At higher speed an instability occurs. At this point any slight shear disturbance in the stress field reverses the relative stability of A– and B–bonds, and the crack is deflected onto a (111) plane. The energy release rate for this system is $G = 6.7$ Jm^{-2}. In addition to the main tensile load, this includes a small $G = 0.24$ Jm^{-2} shear contribution, in order to break the symmetry in the y direction. Both exposed (111) crack surfaces undergo a 2×1 reconstruction. The bottom three panels are photographs from three–point bending experiments[6]. **c**, (110) fracture surface for low–speed cleavage (gray). **d**, Fracture surface of a specimen with the crack deflected from the (110) plane (white) to the (111) plane (black) for intermediate–speed cleavage. **e**, (111) fracture surface obtained for high–speed cleavage.